

# A meron cluster solution for the sign problem of the two-dimensional $O(3)$ model

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## Abstract

The two-dimensional  $O(3)$  model at a vacuum angle  $\theta = \pi$  is investigated. This model has a severe sign problem. By a Wolff cluster algorithm an integer or half-integer topological charge is assigned to each cluster. The meron clusters (clusters with half-integer topological charge) are used to construct an improved estimator for the correlation function of two spins at  $\theta = \pi$ . Only configurations with 0 and 2 merons contribute to this correlation function. An algorithm, that generates configurations with only 0 and 2 merons, is constructed and numerical simulations at  $\theta = \pi$  are performed. The numerical results indicate the presence of long range correlations at  $\theta = \pi$ .

## 1 Introduction

The numerical simulation of many interesting physical systems, including in particular quantum chromodynamics (QCD) at non-zero chemical potential or at non-zero theta vacuum angle, suffers from a complex action problem or a sign problem (see [1] and references therein). The numerical simulation of these systems is impossible with standard Monte Carlo methods. In this article we investigate the two-dimensional  $O(3)$  model at a vacuum angle  $\theta = \pi$ . This model has a severe sign problem. Unlike gauge theories, for which no reliable cluster algorithms are available [15, 16], the  $O(3)$  model can be simulated with the help of cluster algorithms and the meron cluster concept provides a solution of the sign problem. The results obtained in our studies are of interest for the understanding of certain systems in statistical mechanics. Haldane e.g. conjectured [10] that integer and half-integer

one-dimensional antiferromagnetic quantum spin chains behave qualitatively differently. While integer spin chains have a mass gap, half-integer spin chains should be gapless. In the large  $s$  limit ( $2s + 1$  being the number of possible spin orientations) there is a mapping from the one-dimensional antiferromagnetic quantum spin chain on the two-dimensional classical  $O(3)$  model with a  $\theta$  vacuum term [11]. Integer spin chains correspond to  $\theta = 0$  and half-integer spin chains correspond to  $\theta = \pi$ . The  $O(3)$  model at  $\theta = 0$  has a mass gap in agreement with Haldane's conjecture. On the other hand, Haldane's conjecture together with the (non-rigorous) mapping of spin chains on the  $O(3)$  model implies that the mass gap disappears at  $\theta = \pi$ . This corresponds to a phase transition governed by the vacuum angle  $\theta$ .

The paper is organized as follows. In section 2 the Wolff cluster algorithm and the sign problem of the two-dimensional  $O(3)$  model at  $\theta = \pi$  are described. The meron clusters are defined. They are used for the construction of an improved estimator for the correlation function of two spins at  $\theta = \pi$  (section 3). In order to calculate this correlation function a meron cluster algorithm is developed (section 4). The improved estimator together with the meron cluster algorithm will be shown to solve the sign problem. The correlation function at  $\theta = \pi$  is calculated numerically. The results of these calculations are presented in section 5.

## 2 The Wolff cluster algorithm and the sign problem of the two-dimensional $O(3)$ model

The lattice action of the two-dimensional  $O(3)$  model is given by

$$S = -\beta \sum_{\langle xy \rangle} e_x \cdot e_y, \quad \beta > 0. \quad (1)$$

The summation is over all pairs  $\langle xy \rangle$  of nearest neighbor lattice sites. The three-component vectors of unit length are denoted by  $e_x$  and called *spins*. The action has a global  $O(3)$  rotation symmetry.

In numerical simulations of this model one has to generate spin configurations  $\{e\}$  that are distributed with a probability given by the statistical weight factor  $\exp(-S(\{e\}))$ . In the Wolff cluster algorithm [6, 7] some spins are combined and then updated together in one step. For every pair of nearest neighbor lattice sites  $x$  and  $y$  there is a *bond variable*  $b_{xy}$  which only can take the values 0 and 1. If  $b_{xy} = 1$ , one says that  $x$  and  $y$  are connected by

a bond. The bond variables define the *clusters*. A cluster is a set of lattice sites. Lattice sites connected by bonds with each other belong to the same cluster.

The Wolff cluster algorithm consists of the following steps:

1. A vector  $r$  of unit length is chosen whose direction (Wolff direction) is completely random.
2. To generate the clusters, nearest neighbor sites  $x$  and  $y$  are connected with probability

$$p(e_x, e_y) = 1 - \exp(\min[0, -2\beta(e_x \cdot r)(e_y \cdot r)]). \quad (2)$$

(bond activation probability) by a bond. The probability is largest if both spins  $e_x$  and  $e_y$  are aligned parallel or anti-parallel to the Wolff direction  $r$ . It is zero if the projections of the spins on the Wolff direction have different signs.

3. A cluster is flipped with probability  $1/2$  independent of all the other clusters. Cluster flip means that all the spins belonging to the cluster are reflected on the plane perpendicular to the vector  $r$  (Wolff plane)

$$e_x \rightarrow e_x^* = e_x - 2(e_x \cdot r)r. \quad (3)$$

$e_x^*$  denotes the reflected spin.

It has been shown that this algorithm fulfills detailed balance and is ergodic [6, 7].

The spins of the two-dimensional  $O(3)$  model define a mapping from the lattice with periodic boundary conditions to the sphere  $S^2$ . These mappings fall into different classes characterized by an integer valued *topological charge*  $Q$ . For this characterization the spins must be interpolated between the lattice points. The charge  $Q$  counts, how many times the sphere is covered by the mapping. The reason for the existence of the integer valued topological charge  $Q$  is that the homotopy group of continuous mappings from the torus  $T^2$  (the lattice) to the sphere  $S^2$  is isomorphic to the group of integers.

We consider the two-dimensional  $O(3)$  model with an additional topological term in its action

$$S \rightarrow S - i\theta Q. \quad (4)$$

with  $\theta$  real. A complex probability distribution  $\exp(-S)$  does not make sense. For the calculation of expectation values the additional factor  $\exp(i\theta Q)$  must be included in the observable

$$\langle F \rangle \rightarrow \langle \exp(i\theta Q) F \rangle \stackrel{\theta \equiv \pi}{=} \langle (-1)^Q F \rangle. \quad (5)$$

For the special case  $\theta = \pi$  the additional factor becomes  $(-1)^Q$ . The factor  $(-1)^Q$  causes a *sign problem*. In a Monte Carlo calculation the alternating sign  $(-1)^Q$  leads to cancellations between the contributions from different configurations to the expectation value. The numerical calculation of the expectation value is difficult because it has a large variance if  $F$  is one of the usual physical observables.

Using a Wolff cluster algorithm the flip of a cluster changes the topological charge from  $Q$  to  $Q^*$ . We can assign to every cluster a *cluster charge* [8]

$$q = \frac{Q - Q^*}{2} \quad (6)$$

that is either integer or half-integer. Clusters with half-integer charge are called *meron clusters*. Note that the flip of a meron cluster changes the sign  $(-1)^{Q^*} = (-1)^{-2q}(-1)^Q = (-1)(-1)^Q$ . This property of the meron clusters is exploited for the construction of improved estimators at  $\theta = \pi$  (see next section).

### 3 An improved estimator for the correlation function

The numerical calculation of the correlation function  $\langle (-1)^Q e_x \cdot e_y \rangle$  of two spins at  $\theta = \pi$  suffers from large statistical errors because of the sign problem. However the meron clusters can be used to construct an improved estimator (see eq. (9)) for the correlation function. This construction is based on a proposal by U.-J. Wiese.

Because of the  $O(3)$  rotation symmetry it is sufficient to consider the product of the parallel components of the spins (parallel to the Wolff direction). There are two possibilities: Either the lattice sites  $x$  and  $y$  belong to the same cluster  $\mathcal{C}$  or they belong to different clusters

$$\begin{aligned} \langle (-1)^Q e_x^{\parallel} e_y^{\parallel} \rangle = \\ \langle (-1)^Q e_x^{\parallel} e_y^{\parallel} \Theta(\mathcal{C}_x = \mathcal{C}_y) \rangle + \langle (-1)^Q e_x^{\parallel} e_y^{\parallel} \Theta(\mathcal{C}_x \neq \mathcal{C}_y) \rangle. \end{aligned} \quad (7)$$

The symbol  $\Theta(\ )$  is 1 or 0, if the statement in brackets is true or false respectively.  $\mathcal{C}_x$  denotes the cluster that contains the site  $x$ . The flip of a meron cluster changes the sign  $(-1)^Q$ . Therefore when averaging over cluster flips the first term only gets a non-vanishing contribution if the cluster configuration contains no merons. If  $x$  is contained in a meron cluster  $\mathcal{M}_x$  the flip of the meron cluster changes  $(-1)^Q$  and  $e_x^{\parallel}$  simultaneously. Therefore

when averaging over cluster flips the second term only gets non-canceling contributions if  $x$  and  $y$  are both in meron clusters and there are no other meron clusters

$$\begin{aligned} \langle (-1)^Q e_x^\parallel e_y^\parallel \rangle = & \quad (8) \\ \langle (-1)^Q e_x^\parallel e_y^\parallel \Theta(\mathcal{C}_x = \mathcal{C}_y) \Theta(N_{\mathcal{M}} = 0) \rangle + \langle (-1)^Q e_x^\parallel e_y^\parallel \Theta(\mathcal{M}_x \neq \mathcal{M}_y) \Theta(N_{\mathcal{M}} = 2) \rangle. \end{aligned}$$

The factor  $(-1)^Q$  can be removed in both terms on the right hand side. Every cluster configuration can be thought of as being generated by cluster flips from a configuration in which all spins have been on the same side of the Wolff plane. For this configuration  $(-1)^Q = 1$ , because  $Q = 0$ , and  $e_x^\parallel e_y^\parallel > 0$ . The flip of a non-meron cluster does not change  $(-1)^Q$  and  $e_x^\parallel e_y^\parallel$ . The flip of a meron cluster simultaneously changes  $(-1)^Q$  and the sign of  $e_x^\parallel e_y^\parallel$  in the case  $\mathcal{M}_x \neq \mathcal{M}_y$ . Therefore

$$\begin{aligned} \langle (-1)^Q e_x^\parallel e_y^\parallel \rangle = & \quad (9) \\ \underbrace{\langle |e_x^\parallel e_y^\parallel| \Theta(\mathcal{C}_x = \mathcal{C}_y) \Theta(N_{\mathcal{M}} = 0) \rangle}_{=g_{0\mathcal{M}}} + \underbrace{\langle |e_x^\parallel e_y^\parallel| \Theta(\mathcal{M}_x \neq \mathcal{M}_y) \Theta(N_{\mathcal{M}} = 2) \rangle}_{=g_{2\mathcal{M}}}. \end{aligned}$$

With equation (9) the sign problem has turned into the problem of finding cluster configurations with only 0 or 2 merons. Usually cluster configurations contain many merons and configurations with only 0 or 2 merons are quite rare. Therefore one aims at constructing an algorithm that generates only configurations with 0 and 2 merons. Such an algorithm is described in the next section. The improved estimator on the right hand side of equation (9) has no sign problem and therefore enables reliable numerical calculations.

The first term  $g_{0\mathcal{M}}$  only gets non-vanishing contributions from cluster configurations in the zero-meron sector while the second term  $g_{2\mathcal{M}}$  only gets non-vanishing contributions from the two-meron sector. In the term  $g_{0\mathcal{M}}$  the sites  $x$  and  $y$  must be in the same cluster. Therefore, if the distance  $r = r(x, y)$  between the lattice sites  $x$  and  $y$  is much larger than the cluster size, there is no contribution to  $g_{0\mathcal{M}}(r)$ . The decay of  $g_{0\mathcal{M}}(r)$  is known to be mainly governed by the cluster size distribution which is exponential [7]. On the other hand in the term  $g_{2\mathcal{M}}$  the sites  $x$  and  $y$  must be in two different meron clusters. The two meron clusters can be far apart. Then  $g_{2\mathcal{M}}(r)$  gets non-vanishing contributions at large distances  $r$  (large compared to the cluster size). In this way long range correlations can arise.

In figure 1 the correlation functions at  $\theta = 0$  and at  $\theta = \pi$  are compared. This figure shows the slower decay of correlation function at  $\theta = \pi$ .

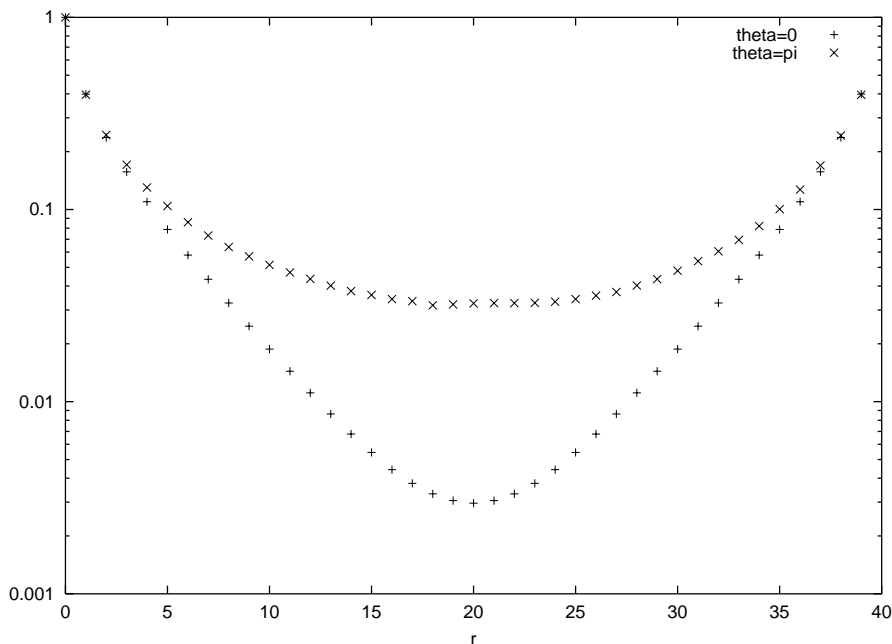


Figure 1: Correlation function at  $\theta = 0$  and at  $\theta = \pi$ .  $L \times L = 40 \times 40$ ,  $\beta = 0.1$ .

## 4 A meron cluster algorithm

Assume that we have a cluster configuration with at most 2 merons. In the Wolff cluster algorithm the Wolff direction, used in the definition of the clusters, is not fixed. After a change of the Wolff direction, however, all bonds become invalid and have to be calculated anew. The new cluster configuration likely contains more than 2 merons.

Thus, a gradual update (that is an update which changes only a few bonds in each step) of the allowed cluster configuration is only possible if the Wolff direction is fixed. In this case the spins are only reflected on a single plane (perpendicular to the Wolff direction). These reflections do not change the spin components perpendicular to the Wolff direction. Therefore the resulting algorithm is not ergodic. To make it ergodic we must combine it with another update step effecting the perpendicular spin components. In this additional step only a few spins and bonds should be updated because we want to make only small changes on the allowed cluster configuration.

For the numerical calculations we use an algorithm with two Wolff directions. Wolff direction 1 is fixed during the whole simulation. The clusters and their charges are defined with respect to this Wolff direction 1. The

cluster flips on the corresponding Wolff plane are not ergodic. To establish ergodicity we use a single cluster algorithm with a Wolff direction 2 that is chosen randomly anew for every update step. In one update step a single cluster is calculated and flipped with respect to the Wolff direction 2. After the single cluster flip the bonds in configuration 1 are calculated anew and the meron number constraint for configuration 1 is checked. If the meron number constraint is violated the single cluster flip is undone and the old bond configuration 1 is restored (accept reject step).

After the single cluster flip only those bonds in configuration 1 are calculated anew whose corresponding spins got changed. Thereby the change of the configuration of spins and bonds induced by the update step is restricted to a relatively small part of the lattice and the acceptance ratio for the update step becomes independent of the lattice size.

With the introduction of a second Wolff direction, the obvious problems with ergodicity are removed. There remains however still the possibility that independent of the details of the algorithm non-ergodic behaviour could arise if certain components of the zero- and two-meron sector are not accessible to our algorithm. It could be that configurations in the zero- and two-meron sector exist which could be reached only from sectors with more than two merons. This would invalidate any approach which deals with selected meron sectors only. We have not been able to rule out this possibility analytically. However we have not found any dependencies on the initial configuration in our results for the correlation function.

## 5 Numerical results

The meron cluster algorithm is used to investigate the large distance behavior of the correlation function of two spins at  $\theta = \pi$ . We calculate the projected correlation function at  $\theta = \pi$

$$g_p(r) = \left\langle (-1)^Q \left( \frac{1}{\sqrt{L_2}} \sum_{x_2=0}^{L_2-1} e_{x_1, x_2}^{\parallel} \right) \left( \frac{1}{\sqrt{L_2}} \sum_{y_2=0}^{L_2-1} e_{y_1, y_2}^{\parallel} \right) \right\rangle \quad (10)$$

(see figure 2) for various values of the lattice size  $L = L_1 = L_2$  at fixed  $\beta = 0.1$ . The spins are summed over one space direction (the 2-direction) in order to suppress the contributions from excited states. This corresponds to a projection on the zero mode. The data points are fitted with a hyperbolic cosine

$$h(r) = A \cosh \left( m_{\pi} \left( \frac{L}{2} - r \right) \right). \quad (11)$$

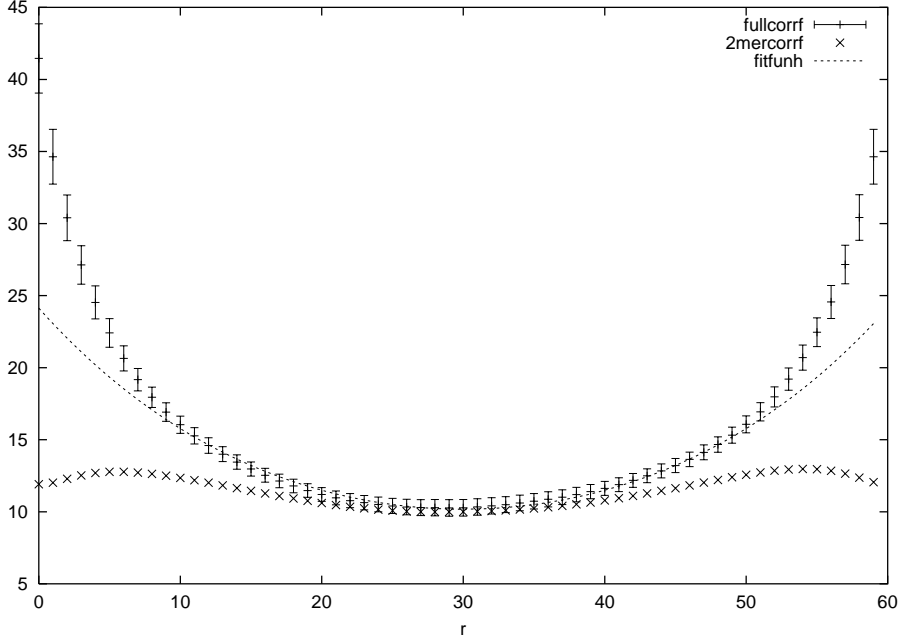


Figure 2: Projected correlation function  $g_p$  and two-meron part of the projected correlation function  $g_{2M,p}$  at  $L = 60$  and  $\beta = 0.1$ .

$A$  and  $m_\pi$  are the fit parameters which must be determined. The  $L$  dependence of the masses  $m_\pi$  obtained in this way is shown in figure 3. The  $L$  dependence of  $m_\pi$  seems to be approximately of the form

$$m_\pi = \frac{C}{L}, \quad C = 3.138. \quad (12)$$

The value of the constant  $C$  is obtained from a fit. These data suggest that in the infinite volume limit the mass  $m_\pi$  vanishes and thus long range correlations are present. The numerical data confirm the conjecture that the correlation function at  $\theta = \pi$  is long ranged (cf. section 3). Also Haldane's conjecture about the behavior of quantum spin chains is supported by the results (cf. section 1).

## 6 Summary

An improved estimator has been defined for the correlation function of two spins in the two-dimensional  $O(3)$  model at  $\theta = \pi$ . A meron cluster algorithm for the numerical calculation of the improved estimator has been developed. The numerical results indicate the occurrence of long range correlations at  $\theta = \pi$ .



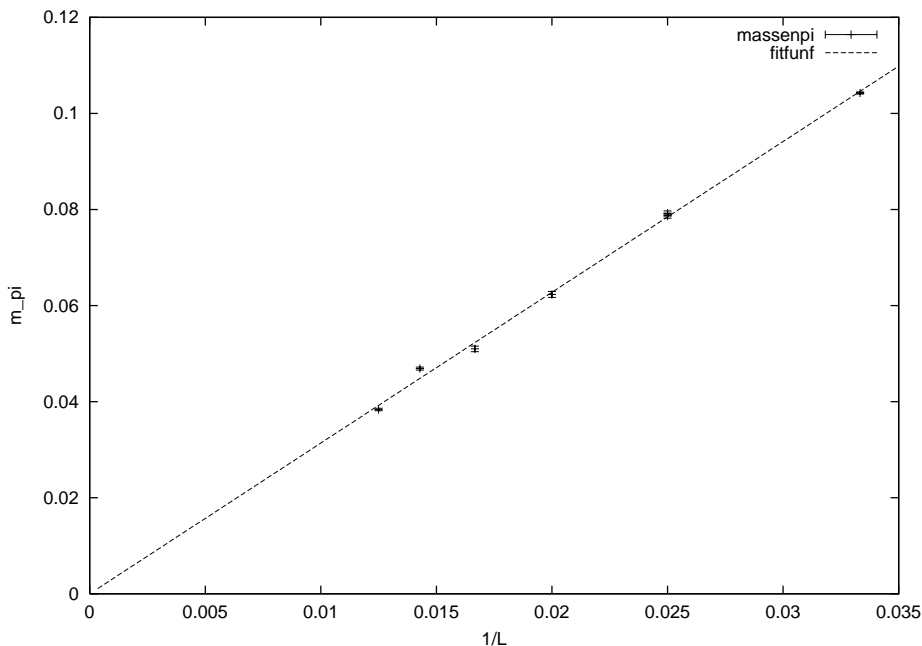


Figure 3: Dependence of the mass  $m_\pi$  on the lattice size  $L$  at fixed  $\beta = 0.1$ . The function  $3.138/L$  is also plotted.

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## References

- [1] M. Alford, S. Chandrasekharan, J. Cox, U.-J. Wiese; hep-lat/0101012
- [2] C. Callan, R. Dashen, D. Gross; Phys. Lett. **B66**, 375 (1977)
- [3] D. Gross; Nucl. Phys. **B132**, 439 (1978)
- [4] E. Witten; Phys. Rev. Lett. **38**, 121 (1977)
- [5] R. Swendsen, J.-S. Wang; Phys. Rev. Lett. **58**, 86 (1987)
- [6] U. Wolff; Phys. Rev. Lett. **62**, 361 (1989)
- [7] U. Wolff; Nucl. Phys. **B334**, 581 (1990)

- [8] W. Bietenholz, A. Pochinsky U.-J. Wiese; Phys. Rev. Lett. **75**, 4524 (1995)
- [9] S. Chandrasekharan, U.-J. Wiese; Phys. Rev. Lett. **83**, 3116 (1999); cond-mat/9902128
- [10] F. Haldane; Phys. Lett. **A93**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983)
- [11] I. Affleck; Nucl. Phys. **B257**, 397 (1985)
- [12] G. Bhanot, R. Dashen, N. Seiberg, H. Levine; Phys. Rev. Lett. **53**, 519 (1984)
- [13] I. Montvay, G. Münster; Quantum Fields on a Lattice; Cambridge University Press, 1994
- [14] J. Kogut; Rev. Mod. Phys. **51**, 659 (1979)
- [15] K. Jansen, U.-J. Wiese; Nucl. Phys. **B370**, 762 (1992)
- [16] S. Caracciolo, R. Edwards, A. Pelissetto, A. Sokal; hep-lat/9205005